An International Journal of Optimization and Control: Theories & Applications
ISSN: 2146-0957 eISSN: 2146-5703
Vol.16, No.3, pp.1049-1063 (2026)
https://doi.org/10.36922/IJOCTA026040011

RESEARCH ARTICLE

Integration of topological indices and QSPR modeling with VIKOR-based multi-criteria decision analysis for evaluating eye drug candidates

Muhammad Kamran[1,2,3†], Shereen Iqbal[4†], Hifza Iqbal[4*], Muhammad Akhtar Tarar[5†], Muhammad Farman[1,6], Evren Hincal[1,7] and Mohamad Hafez[3,8]

[1]Mathematics Research Center, Department of Mathematics Near East University, Mersin, Turkey
[2]International Center for Interdisciplinary Research in Sciences, The University of Lahore, Lahore, Pakistan
[3]Department of Mathematics, Faculty of Engineering and Quantity Surviving, INTI International University Colleges, Nilai, Negeri Sembilan, Malaysia
[4]Department of Mathematics and Statistics, The University of Lahore, Lahore, Punjab, Pakistan
[5]Department of Civil Engineering, The University of Lahore, Lahore, Punjab, Pakistan
[6]Department of Computer Engineering, Biruni University, Istanbul, Turkey
[7]Research Center of Applied Mathematics, Khazar University, Baku, Azerbaijan
[8]Department of Management, Faculty of Management, Shinawatra University, Pathum Thani, Thailand
kamrankfueit@gmail.com; shereeniqbal321@gmail.com; iqbalhifza3@gmail.com; akhtartarar2000@yahoo.com; farmanlink@gmail.com; evren.hincal@neu.edu.tr; mohdahmed.hafez@newinti.edu.my

ARTICLE INFO

Article History:
Received: January 19, 2026
Revised: March 12, 2026
Accepted: March 19, 2026
Published Online: May 13, 2026

Keywords:
Graph theory
Multi-criteria decision-making
Multiple linear regression
Public health
Quantitative structure–property relationship ranking
VIKOR

AMS Classification 2010:
26A33; 34A08; 35H15; 34K50 47H10; 60H10

ABSTRACT

Topological indices encode molecular structure into numerical descriptors, enabling prediction of physicochemical properties without extensive experimentation. This study evaluates the implementation of graph-theoretical topological indices in combination with multi-criteria decision-making methods to compute physicochemical properties and ranking of eye drugs. A set of classical topological indices, consisting of NSK_1, NSK_2, M_1, M_2, NM_1, NM_2, NSK, NF, and NH, are computed using an edge-partition approach to describe the structural aspects of 12 selected drugs. Multiple linear regression models were developed to develop quantitative structure–property relationship models for important physicochemical properties, including molar volume, polarizability, molar weight, and molar refraction. The multiple linear regression models showed reliable predictive output, with statistical indicators and correlation coefficients higher than 0.89, confirming the value of the selected indices. The VIKOR technique enables the ranking of drugs based on their estimated physicochemical properties. The combined application of quantitative structure–property relationship and multi-criteria decision-making framework enhances robustness in discriminating structurally similar eye drugs. This combination offers a systematic framework for prioritizing compounds in pharmacological research and drug optimization. Such approach also supports public health by facilitating more efficient drug development and therapeutic decision-making for eye diseases.

*Corresponding Author
†*These authors contributed equally to this work.*

1. Introduction

A wide range of eye disorders encompasses conditions that effect vision and eye health, ranging from mild, manageable problems to serious diseases that can impair sight.[1] Notably, progressive clouding of the ocular lens, known as cataract, is the most prevalent condition, resulting in limited sight. The therapeutic approach involves implantation of a synthetic intraocular lens[2] after removal of the affected lens. Glaucoma is one of the most serious eye disorder, which is a set of clinical conditions linked to degeneration of optic nerves. This disorder is commonly caused by an increase in pressure within the eye. Patients with glaucoma commonly report complaints such as blurred vision, discomfort in the eyes, restriction of peripheral vision, and a progressive decline in eyesight.[3] Glaucoma is treated clinically by reducing intraocular pressure using pharmacological therapy to prevent progressive optic nerve damage, as well as through laser-based interventions.[4]

Age-related oracular degeneration is recognized as a major cause of vision loss in elderly individuals. This disorder arises from the degeneration of central retina and is commonly demonstrated by blind spots, challenges in reading, and visual distortion [5]. Current treatment techniques, including photo-dynamic therapy, anti-vascular endothelial growth factor injections, and laser interventions, are primarily aimed at delaying disease propagation and preserving remaining vision. Diabetic eye disease, a well-known micro vascular disorder, develops due to retinal blood vessel damage. Symptoms may include progressive eyesight loss, floaters, and blurred vision.[6] Conjunctivitis, commonly known as pink eye, is an inflammatory condition affecting the thin, translucent membrane that covers the sclera and lines the inner surface of the eyelids. [7]. Its clinical manifestation include eyelid crusting, itching, redness, discharge, and tearing.[8] Allergic conjunctivitis is treated with supportive techniques such as cold compresses and antihistamine drops, whereas bacterial conjunctivitis is usually cured by antibiotic eye drops.[9]

A collection of eye drugs plays an important role in eye ailments management by using various pharmacological techniques. Carbolic anhydrase modulating agents such as acetazolamide,[10] and brinzolamide[11] lower intraocular pressure proficiently, thereby contributing to glaucoma supervision and reducing aqueous humor secretion. Acetylcysteine [12] acts as an antioxidant for dry eye conditions, thereby improving corneal health in inflammatory keratitis, while aciclovir[13] and ganciclovir [14] serve as antiviral agents against human cytomegalovirus diseases. Tropicamide[15] and cyclopentolate,[16] both parasympathetic drugs, are commonly used for indicative cyclopedia and mydriasis. xylometazoline,[17] and apraclonidine,[18] act to alleviate eye congestion. Adrenergic receptor agonists decrease intraocular pressure by decreasing aqueous humor production and inducing vasoconstrictive effects on ocular blood vessels. Bromfenac,[19] a nonsteroidal anti-inflammatory drug, effectively controls postoperative inflammation following ocular surgery. Carteolol,[20] a β-blocker, reduces intraocular pressure with minimal systemic effects, while lodoxamide[21] stabilizes mast cells thereby preventing allergic conjunctivitis. These drugs form a dynamic part of modern pharmacotherapy, targeting infectious, inflammatory, and pressure-related ocular diseases with high therapeutic precision. This is supported by studies highlighting the impact of infection and parasitic diseases on self-rated health, as well as the role of socioeconomic and environmental factors, including housing conditions, in the spread and mitigation of infection diseases.[22,23]

Euler, in 1736 first formulated graph theory by constituting a fundamental branch of discrete mathematics.[24,25] Since its inception, it has found widespread use in technological fields, such as chemistry, physics, biology, and computer science, and in multiple scientific techniques.[26,27] The development of chemical graph theory has emerged through the integration of molecular structures with mathematical frameworks. The main purpose of this field lies in the study of topological indices, which perform as numerical tools strongly correlated with the functional and structural properties of molecules. These indices are widely applied in quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) modeling, where they provide a reliable basis for predicting biological activities and physicochemical properties of chemical entities.[28]

Topological indices act as mathematical tool that efficiently capture the structural properties of chemical compounds.[29] The concept of topological indices was first introduced through the Wiener index in 1947, which played a pioneer role in correlating physicochemical properties with the molecular structure of petroleum.[30] Since then, in chemical graph theory, these indices have become fundamental tools, enabling the analysis and calculation of physicochemical properties. A molecular graph G is constructed from the structural framework of hydrocarbons. In such graph, the

vertices correspond to atoms other than hydrogen, and this set of collection is depicted as $V(G)$. The bonds between these atoms are represented as edges, and set of edges is denoted by $E(G)$.[31,32]

The first and second Zagreb indices, originally proposed by Trinajsti and Gutman,[33] are among the earliest and most fundamental topological descriptors in chemical graph theory. These indices have since played a pivotal role in correlating molecular structure with various physicochemical and biological properties.

Mathematically, these indices are expressed as:

$$M_1(G) = \sum_{ab \in E(G)} d(a) + d(b), \tag{1}$$

$$M_2(G) = \sum_{ab \in E(G)} d(a) \times d(b), \tag{2}$$

where $d(a)$ and $d(b)$ represent the degrees of vertices a and b, respectively.

$$NM_1(G) = \sum_{ab \in E(G)} \left[S(a) + S(b)\right], \tag{3}$$

$$NM_2(G) = \sum_{ab \in E(G)} \left[S(a) \times S(b)\right], \tag{4}$$

where $S(a)$ and $S(b)$ represent the sum of neighborhood degrees of vertices a and b, respectively. The Hyper Zagreb index, denoted as $HM(G)$, [34] is mathematically defined as follows:

$$HM(G) = \sum_{ab \in E(G)} (d(a) + d(b))^2 \tag{5}$$

Shirdel et al. proposed a revised formulation of the Zagreb indices.[35] In this modification, the expression for the second Zagreb index of a graph G is reformulated as follows:

$$ReZG_2(G) = \sum_{ab \in E(G)} \frac{d(a) \times d(b)}{d(a) + d(b)} \tag{6}$$

The square root maximum–minimum degree index $mMsde(G)$ is defined as:

$$mMsde(G) = \sum_{ab \in E(G)} \sqrt{\frac{\max\{d(a), d(b)\}}{\min\{d(a), d(b)\}}} \tag{7}$$

The neighborhood Sombor–Kulli NSK index is defined as:

$$NSK(G) = \sum_{ab \in E(G)} \sqrt{S(a)^2 + S(b)^2} \tag{8}$$

The SK_1 index (first Sombor-type index) is described as:

$$SK_1(G) = \sum_{ab \in E(G)} \frac{1}{\sqrt{d(a)^2 + d(b)^2}} \tag{9}$$

The SK_2 index (second Sombor-type index) described as:

$$SK_2(G) = \sum_{ab \in E(G)} \sqrt{d(a)^2 + d(b)^2} \times [d(a) + d(b)] \tag{10}$$

The neighborhood harmonic index is defined as:

$$NH(G) = \sum_{ab \in E(G)} \left[d(a)^2 + d(b)^2\right] \tag{11}$$

The neighborhood forgotten index is defined as:

$$NF(G) = \sum_{b \in V(G)} d(b)^3 \tag{12}$$

Topological indices for the compounds depicted in **Figure 1** were derived using an edge partitioning approach. In this method, the indices are computed by systematically counting edges that join vertices with the same degree classification $(d(a), d(b))$.

2. Methodology

This study employed a combined computational framework integrating graph-theoretical topological indices, QSPR modeling, and multi-criteria decision-making (MCDM) analysis. Molecular structures of 12 ophthalmic drug candidates were initially retrieved from established pharmacological databases and translated into molecular graphs, where atoms represent vertices and bonds represent edges. A set of classical and newly defined topological descriptors $M_1, M_2, NM_1, NM_2, NSK, NSK_1, NSK_2, NH$, $NF, HM, mMsde$, and $ReZG_2$ was calculated using an edge-partitioning algorithm. Subsequently, a multiple linear regression (MLR) analysis was performed to develop QSPR models correlating these descriptors with experimental physicochemical parameters, including polarizability, molar volume, molar refraction, and molecular weight. Statistical metrics, including correlation coefficient, coefficient of determination, Fisher's statistic, standard error, and root mean square error were used to evaluate model performance and predictive accuracy. For MCDM, the VIKOR method was used based on their predicted physicochemical behavior to prioritize the studied drugs. The topological indices and weights assigned to these indices served as decision criteria, which enable compromise-based ranking of drugs that identified the most structurally efficient candidates.

Figure 1 depicts the molecular structures of the 12 drugs for ocular disorders analyzed in this study. These chemical structures serve as the foundation for constructing molecular graphs

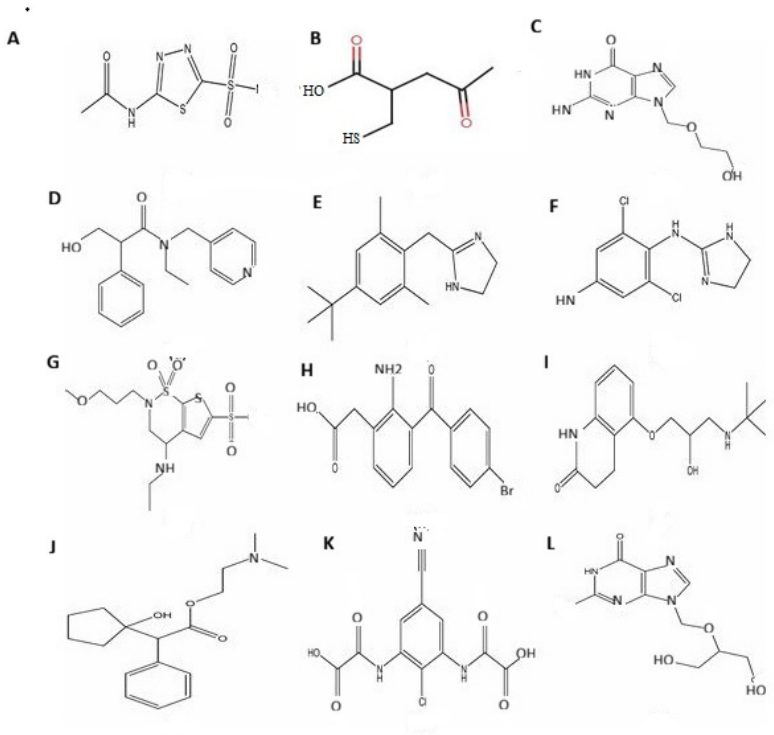

Figure 1. Molecular structure of (A) acetazolamide, (B) acetylcysteine, (C) aciclovir, (D) tropicamide, (E) xylometazoline, (F) apraclonidine, (G) brinzolamide, (H) bromfenac, (I) carteolol, (J) cyclopentolate, (K) lodoxamide, and (L) ganciclovir

Table 1. Physicochemical properties of ophthalmic drugs

Eye drugs	Polarizability	Molar volume	Molar refraction	Molar weight
Acetylcysteine	15.2	126.1	38.3	163.2
Acetazolamide	18.9	110.6	47.7	222.3
Aciclovir	20.8	127.2	52.4	225.2
Apraclonidine	23.5	150	59.2	245.11
Tropicamide	32.6	244.8	82.2	284.35
Bromfenac	31.4	213.5	79.1	334.16
Brinzolamide	35.8	255.4	90.4	383.5
Cartelol	32.3	258.6	81.4	292.3
Iodoxamide	26	174.6	65.5	311.63
Cyclopentolate	32.7	256.5	82.4	291.4
Ganciclovir	23	140.6	57.9	255.23
Xylometazoline	30.5	243.6	76.9	244.37

used to compute topological indices. Each chemical structure reflects a distinct atomic connectivity and arrangement, which influence its physicochemical properties and ranking.

Table 1 presents the experimentally obtained physicochemical parameters–polarizability, molar volume, molar refraction, and molecular weight—of the selected drugs, sourced from PubChem. These physicochemical parameters provide insight into molecular size, optical properties, and inter molecular interactions of compounds, serving as dependent variables in the QSPR modeling framework.

Multiple linear regression is a most commonly used technique for predicting a target variable based on two or more independent variables. [36] The mathematical form of multiple linear regression model is:

$$Z = a_1 I_1 + a_2 I_2 + a_3 I_3 + \cdots + k,$$

where Z denotes the target variable, a_i represents the coefficients of regression corresponding to the input variables I_i, and k is known as regression constant. In MLR framework, several modeling approaches have been developed, including

step-wise regression, the standard method, sequential forward selection, and sequential backward approach. In this study, the standard method was employed, where physicochemical properties served as target variables, while topological indices served as input variables. To evaluate model performance, key statistical metrics were employed, including sample size (n), correlation coefficient (r), standard error, coefficient of determination (R^2), Fisher's statistic (F), and significance level (p). These metrics describe the reliability and predictive capacity of the regression model.

3. Results and discussion

This section integrates topological indices with MCDM methods and QSPR gives a systematic approach for quantitative drug validation. The high degree of correlation between the physicochemical properties and computed indices underscores the structural interpretability of these indices. Topological indices such as NM_1, NH, and NSK effectively captured structural topology that influenced major physicochemical attributes relevant to eye drugs design.

Illustrative computation:

Let G represent molecular graph of acetylcysteine, then

$M_1 = 40,\ M_2 = 41,\ NM_1 = 238,\ NM_2 = 216,\ NSK = 212,\ NSK_1 = 534,\ NSK_2 = 610, NH = 620,\ NF = 479,\ mMsde = 13.02,\ HM = 184,\ and\ ReZG_2 = 8.77.$

Based on **Figure 1**, $|V(G)| = 9$ and $|E(G)| = 9$. Degree-based edge partitions of acetylcysteine are as follow:

$$E_{3,4} = \{e = ab \in E(G) \mid d(a) = 3,\ d(b) = 4\},$$
$$E_{3,5} = \{e = ab \in E(G) \mid d(a) = 3,\ d(b) = 5\},$$
$$E_{4,6} = \{e = ab \in E(G) \mid d(a) = 4,\ d(b) = 6\},$$
$$E_{4,7} = \{e = ab \in E(G) \mid d(a) = 4,\ d(b) = 7\},$$
$$E_{5,7} = \{e = ab \in E(G) \mid d(a) = 5,\ d(b) = 7\},$$
$$E_{6,7} = \{e = ab \in E(G) \mid d(a) = 6,\ d(b) = 7\}.$$

such that $|E_{3,4}| = 3$, $|E_{3,5}| = 2$, $|E_{4,6}| = 1$, $|E_{4,7}| = 1$, $|E_{5,7}| = 1$, and $|E_{6,7}| = 1$.

The required results were obtained using **Equations 1–12**.

Similarly, the results for the remaining drugs are summarized in **Table 2**.

The predictive performance of the topological indices in modeling molecular activity was validated using the MLR models, which demonstrated satisfactory accuracy in estimating physicochemical properties. The potential of these models as computational substitutes for preliminary screening is supported by the agreement between predicted and observed values. An additional decision-support approach based on VIKOR method was introduced to integrate multiple physicochemical parameters into a single evaluation model. Evidence-based drug candidate selection was facilitated by the resulting framework, which showed differences between structurally isomorphic molecules. Brinzolamide obtained a lower ranking due to its complex structure and higher molecular weight, while acetylcysteine's ranking at the top can be attributed to its balanced molecular characteristics and favorable physicochemical profile.

Overall, the combined QSPR–VIKOR approach shows a successful strategy for selection in ophthalmic research and rational drug ranking. It not only provides a reproducible mathematical foundation for early-phase drug screening but also reduces dependency on experimental assays. Future studies may incorporate additional graph descriptors, larger molecular datasets, and advanced machine-learning approaches for generalization across drug classes and to further enhance predictive accuracy.

Table 2, presents the quantitative measures of the computed graph-theoretical indices ($NSK, NSK_1, NSK_2, M_1, M_2, NH, NF, NM_1, NM_2, mMsde, ReZG_2$, and HM) for every drug. The diversity in these values captures variations in molecular topology, which are crucial for correlating structure with properties. **Table 3** presents the correlation coefficients between the topological indices and the measured physicochemical properties. The consistently high correlation values ($r \geq 0.89$) affirm that the chosen descriptors accurately reflect structural influence on the compounds' physicochemical characteristics.

3.1. Regression models

(a) Model 1

$P = -4.3447 + 0.6661(mMsde) - 1.4494(ReZG_2) + 0.3203(NM_1) - 0.0562(NM_2) + 3.3858(NH)$

$n = 12,\ F = 10.1165,\ p = 0.0069,\ R = 0.9455,\ R^2 = 0.894,\ SE = 30.65,\ VIF = 4.9809.$

(b) Model 2

$\mathrm{MV} = -36.0271 + 16.7369(M_1) - 9.2227(M_2) -$

Table 2. Topological indices of ophthalmic drugs

Eye drugs	M_1	M_2	NM_1	NM_2	NSK	NSK_1	NSK_2	NH	NF	$mMsde$	HM	$ReZG_2$
Acetazolamide	60	70	140	383	70	191.5	392	2.53	802	18.97	322	13.81
Acetylcysteine	40	41	83	195	41.5	97.5	202.25	2.06	419	13.02	184	8.77
Aciclovir	80	93	186	534	93	267	545	3.39	1,112	20.45	388	19.07
Tropicamide	100	114	228	610	114	305	626	4.53	1,286	25.36	470	24.08
Xylometazoline	96	114	216	620	108	310	634.5	3.46	1,298	24.68	496	21.96
Apraclonidine	76	87	174	479	87	239.5	489	3.04	998	19.99	368	17.85
Brinzolamide	106	125	284	886	142	443	910.5	4.56	1,876	28.45	556	23.75
Bromfenac	96	109	224	606	112	303	623	4.11	1,280	24.10	452	23.05
Cartelol	106	118	254	706	127	353	722	4.29	1,478	28.90	520	24.03
Cyclopentolate	104	119	238	676	119	338	697.5	4.38	1,438	27.08	510	24.23
Iodoxamide	90	101	216	590	108	295	605.5	3.86	1,242	25.47	438	20.45
Ganciclovir	90	105	212	609	106	304.5	625	3.65	1,282	23.54	440	21.33

Table 3. Correlation values of various indices for different properties of ophthalmic drugs

Property	M_1	M_2	NM_1	NM_2	NSK	NSK_1	NSK_2	NH	NF	$mMsde$	$ReZG_2$	HM
Polarizability	0.9275	0.9172	0.9208	0.8891	0.9208	0.8891	0.8909	0.9208	0.8929	0.9116	0.9081	0.9225
Molar volume	0.8333	0.8109	0.8043	0.7659	0.8043	0.7659	0.7683	0.8234	0.7713	0.8274	0.8013	0.9225
Molar refraction	0.9268	0.9167	0.9206	0.8893	0.9206	0.8893	0.8911	0.9202	0.8930	0.9113	0.9072	0.9222
Molar weight	0.8123	0.8051	0.8845	0.8773	0.8845	0.8773	0.8796	0.8582	0.8815	0.8397	0.7882	0.8183

$3.8381(NM_1) + 1.6575(NSK_1)$
$n = 12$, $F = 5.2851$, $p = 0.0279$, $R = 0.8667$, $R^2 = 0.7512$, $SE = 36.94$, $VIF = 2.29516$.

(c) Model 3

$\mathrm{MR} = 7.1373 + 1.1012(NSK) - 1.6544(NSK_2) + 0.7702(NF) - 0.3407(mMsde)$
$n = 12$, $F = 14.695$, $p = 0.001$, $R = 0.9453$ $R^2 = 0.8936$, $SE = 6.77$, $VIF = 4.9632$.

(d) Model 4

$\mathrm{MW} = 127.3426 - 0.2588(HM) - 4.7906(NM_2) + 5.1019(NSK_2)$
$n = 12$, $F = 12.1937$, $p = 0.002$, $R = 0.9058$, $R^2 = 0.8206$, $SE = 28.83$, $VIF = 3.0617$.

Topological indices are not selected randomly; intially, these indices were screened using correlation analysis. Only those indices which show strong correlation coefficients ($|r| \geq 0.70$) with the target physicochemical property were considered for model construction. Subsequently, MLR models were developed using step-wise selection to retain only statistically significant descriptors ($p < 0.05$).

To examine the presence of multicollinearity among the selected descriptors, the variance inflation factor (VIF) was calculated for each independent variable. In the present study, the calculated VIF values for all selected topological indices, fall within the acceptable range, as shown in **Table 4**. This suggests that the independent variables do not exhibit strong inter correlations. It further indicates that each index contributes to the regression model and that the estimated coefficients of models are reliable. Therefore, the developed models can be considered free from significant multicollinearity effects and statistically stable.

Table 5 presents the predicted values of the physicochemical properties obtained through MLR models. The close agreement between predicted and observed values as described in **Tables 1** and **5** validates the robustness and generalizability of the developed QSPR models.

Figure 2 compares the actual and estimated physicochemical parameters graphically. The near-overlapping data trends confirm that the QSPR models effectively capture the relationship between molecular structure and hysicochemical properties.

3.2. Multi-criteria decision-making technique

Multi-criteria decision-making refers to a systematic approach used to analyze and resolve decision-making and planning problems that incorporate multiple evaluation criteria.[37,38] In many real-world cases, a single optimal solution may not exist; therefore, decision makers must differentiate among alternatives based on their preferences and objectives.[39] The notion of solution in this context can vary; it may imply

Table 4. Variation inflation factor values of various indices for different properties of ophthalmic drugs

Property	M_1	M_2	NM_1	NM_2	NSK	NSK_1	NSK_2	NH	NF	$mMsde$	$ReZG_2$	HM
Polarizability	7.153	6.297	6.570	4.773	6.570	4.773	4.874	6.570	4.933	5.917	5.701	6.711
Molar volume	3.272	2.919	2.832	2.418	2.831	2.418	2.441	3.105	2.468	3.170	2.794	6.711
Molar refraction	7.090	6.263	6.557	4.781	6.557	4.781	4.855	6.526	4.893	5.898	5.650	6.686
Molecular weight	2.939	2.842	4.594	4.341	4.594	4.341	4.419	3.795	4.485	3.391	2.640	3.026

Table 5. Estimated values of physicochemical properties of selected ophthalmic drugs

Eye drugs	**Polarizability**	**Molar volume**	**Molar refraction**	**Molar weight**
Acetazolamide	20.15	102.69	46.93	209.15
Acetylcysteine	13.02	98.36	36.51	177.41
Tropicamide	31.16	216.73	78.85	277.23
Aciclovir	22.68	173.88	57.39	249.28
Apraclonidine	22.22	156.01	55.78	232.23
Brinzolamide	34.23	187.43	87.75	384.25
Bromfenac	29.89	200.44	77.42	285.74
Carteolol	34.16	209.91	81.02	294.17
Lodoxamide	28.12	176.37	72.23	276.73
Ganciclovir	26.42	173.27	69.24	284.68
Cyclopentolate	31.63	213.84	82.55	315.48
Xylometazoline	26.32	204.12	67.66	265.96

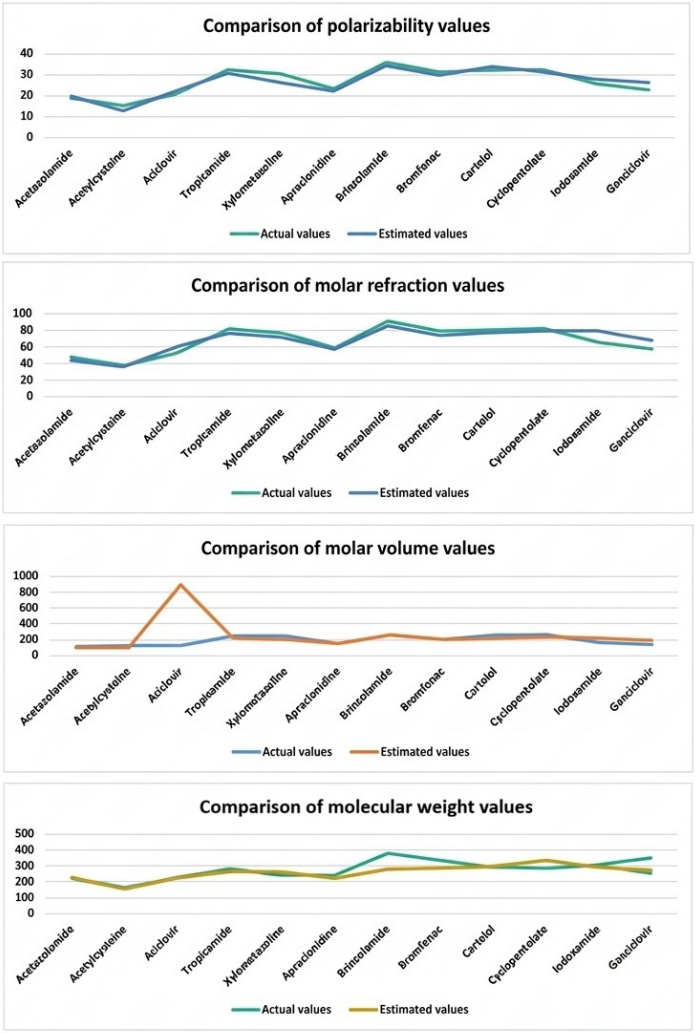

Figure 2. Comparison of actual and estimated values of physicochemical properties

selecting the most preferred option from a set of alternatives, identifying a subset of practical choices, or ranking them according to priority. In its broadest sense, MCDM aims to determine all efficient or non-dominated alternatives that best satisfy the established criteria.[36]

The QSPR approach, integrated with the VIKOR method, offers a systematic framework for assessing and prioritizing compounds based on their biological and pharmacological characteristics.[37] MCDM technique, VIKOR,[38] was employed to rank 12 ophthalmic drugs. In this method, the weighting factors were determined through the ratio approach **(Figure 3)**, and a comparable procedure was followed for assigning weights to other molecular properties.

3.3. VIKOR technique

In order to obtain results that approach the optimal solution, the VIKOR technique was applied. This method considers each investigated drug as an alternative and evaluates them using a set of predefined criteria derived from the QSPR analysis conducted in this study. By combining multiple criteria, VIKOR enables systematic comparison of alternatives and provides a statistically supported ranking of the drugs. Crucially, the method identifies a solution that approximates the optimal result, showing a balanced trade-off between conflicting factors and providing insight for decision-making in drug prioritization. Zeleny[39] proposed the notion of compromise-based solutions within MCDM with practical applications identified in 1998.[40] The following algorithm explained the proposed methodology steps, which are described as follows:

[H] VIKOR algorithm Decision matrix f_{ij}, weight vector w_i, compromise parameter $v \in [0,1]$ S_j, R_j, Q_j and final ranking

Initialize parameters

Determine number of alternatives m and criteria n

$i = 1\ n$ Determine the best value:

$$f_i^+ = \begin{cases} \max_j f_{ij}, & \text{if criterion } i \text{ is benefit type} \\ \min_j f_{ij}, & \text{if criterion } i \text{ is cost type} \end{cases}$$

Determine the worst value:

$$f_i^- = \begin{cases} \min_j f_{ij}, & \text{if criterion } i \text{ is benefit type} \\ \max_j f_{ij}, & \text{if criterion } i \text{ is cost type} \end{cases}$$

$j = 1\ m$ Compute the utility measure:

$$S_j = \sum_{i=1}^{n} w_i \frac{f_i^+ - f_{ij}}{f_i^+ - f_i^-}$$

Compute the regret measure:

$$R_j = \max_i \left[w_i \frac{f_i^+ - f_{ij}}{f_i^+ - f_i^-} \right]$$

Determine:

$$S^+ = \min_j S_j, \quad S^- = \max_j S_j$$

$$R^+ = \min_j R_j, \quad R^- = \max_j R_j$$

$j = 1\ m$ Compute the VIKOR index:

$$Q_j = v \frac{S_j - S^+}{S^- - S^+} + (1 - v) \frac{R_j - R^+}{R^- - R^+}$$

Rank alternatives in ascending order of Q_j

Select the best alternative based on minimum Q_j and check VIKOR acceptance conditions

The relative weight w_i of each criteria is calculated by dividing its mean by the sum of all criterion means:

$$w_i = \frac{\bar{Y_i}}{\sum_{k=1}^{m} \bar{Y_k}},$$

where m is the number of criteria. This ensures:

$$\sum_{i=1}^{m} w_i = 1$$

Table 6 presents the results considering polarizability as the evaluation criterion, with relative importance assigned to each topological index. The assign weights are evenly distributed, which shows that, in prediction of polarizability, no single index dominates. However, indices such as M_1, HM , and NH contributes slightly higher, suggesting that overall cumulative neighborhood effects and molecular connectivity play a remarkable role in determining the susceptibility to polarization of ophthalmic drugs.

The weights described in **Table 7** reflect the sensitivity of molar volume to molecular structure. In defining molecular size, the HM index gains the highest weight, emphasizing the role of vertex connectivity. Indices such as M_1 and $mMsde$ also contribute significantly, indicating that variations in degree distribution that affect the volumetric occupation. The indices NSK_1 and NM_2 gained relatively lower weights, implying that extreme neighborhood interactions have a reduced impact on volumetric behavior.

Table 8, presents the weight distribution across indices, indicating that molar refractivity depends on a combination of neighborhood interactions, branching, and overall connectivity. Higher weight values associated with HM, M_1, and NM_1 suggest that degree-based interactions and molecular compactness influence optical response. Based on **Table 9**, indices related to

Table 6. Weights allocated for polarizability

M_1	M_2	NM_1	NM_2	NSK	NSK_1	NSK_2	NH	NF	$mMsde$	$ReZG_2$	HM
0.08501	0.08407	0.08440	0.08150	0.08440	0.08150	0.08166	0.08440	0.08184	0.08357	0.08325	0.08456

Table 7. Weights allocated for molar volume

M_1	M_2	NM_1	NM_2	NSK	NSK_1	NSK_2	NH	NF	$mMsde$	$ReZG_2$	HM
0.08601	0.08367	0.08298	0.07906	0.08298	0.07906	0.07930	0.08500	0.07963	0.08541	0.08267	0.09523

Table 8. Weights allocated for molar refractivity

M_1	M_2	NM_1	NM_2	NSK	NSK_1	NSK_2	NH	NF	$mMsde$	$ReZG_2$	HM
0.08497	0.08404	0.08440	0.08153	0.08440	0.08153	0.08170	0.08436	0.08187	0.08354	0.08316	0.08458

Table 9. Weights allocated for molecular weight

M_1	M_2	NM_1	NM_2	NSK	NSK_1	NSK_2	NH	NF	$mMsde$	$ReZG_2$	HM
0.07956	0.07890	0.08666	0.08596	0.086666	0.08596	0.08618	0.08407	0.08637	0.08228	0.07722	0.08031

cumulative degree effects and neighborhood size, particularly NSK, NM_1, and NF, gain slightly higher weights, indicating that molecular weight is sensitive to the total structural mass within the graph rather than edge variations. The contribution of M_1 and M_2 suggest that simple degree sums are insufficient to capture molecular weight differences among the studied drugs.

Figure 3, illustrates the influence of physical and chemical properties used in VIKOR analysis. The balanced weighting among polarizability, molecular weight, molar volume, and refractivity shows that selected properties contribute significantly to the decision-making process.

Table 10 summarizes the ranking of drugs used for ocular treatment according to polarizability. Acetylcysteine highlighted as the top-ranked drug, reflecting its favorable balance between ideal and worst-case solutions. Conversely, brinzolamide gains the lowest rank, which can be associated to its variation from the ideal values of polarizability within the evaluated data set.

The results in **Table 11** describe a similar pattern, with acetylcysteine again achieved the top position due to its best adjustment between structural efficiency and molecular size. Acetazolamide and apraclonidine gain relatively strong rankings, while compounds with large molecular structures, such as cyclopentolate and brinzolamide, are placed at the lower end. This result implies that larger molar volume that may decrease suitability under the selected evaluation criteria. **Table 12**, demonstrates that in terms of molar refractivity drugs with moderate structural complexity tend to give better outcome. Because of stable optical behavior of acetylcysteine consistently gains first rank across properties. Apraclonidine and aciclovir also exhibit favorable rankings, whereas brinzolamide again appears at the lower rank, showing less refractive properties relative to other drugs.

The results presented in **Table 13** highlight the influence of molecular weight on drug ranking. Compounds with lower molecular weight and efficient structural distribution, particularly acetazolamide and acetylcysteine, achieve superior ranks. Molecules with higher molecular weight, including carteolol and brinzolamide, are ranked lower, which may adversely affect pharmaceutical behavior of these drugs.

Figure 4 displays a visual comparison of overall VIKOR rankings in accordance with all physicochemical criteria. The consistency observed in the drug positions highlights the stability of the applied decision-making technique. Acetylcysteine consistently stands out as the most favorable drug, while brinzolamide occupies the lowest rank. This visualization increase the valuable results and supports the credibility of integrated QSPR–VIKOR framework.

Table 14 presents the final rankings obtained by evaluating properties into a combined decision matrix. The results in the table show favorable constancy across molar volume, polarizability, molecular weight, and molar refractivity. Acetylcysteine obtains the top rank position across all criterion, indicating a well-balanced physicochemical properties. Acetylcysteine consistently gains firs rank because of its simple and compact molecular structure produces balanced degree distributions. Its low molecular weight and limited structural complexity lead to enhance efficacy as

Table 10. VIKOR ranking of ophthalmic drugs based on polarizability

Ophthalmic drugs	S_j	R_j	Q_j	**Polarizability rank**
Acetazolamide	0.296179	0.031369	0.3264008	2
Acetylcysteine	0.000000	0.000000	0.000000	1
Aciclovir	0.464481	0.055467	0.5473903	4
Tropicamide	0.763575	0.083391	0.8552645	9
Xylometazoline	0.740913	0.081028	0.8309866	8
Apraclonidine	0.4620425	0.048896	0.5089676	3
Brinzolamide	0.995244	0.085010	0.9813049	12
Bromfenac	0.7179826	0.076899	0.7959829	7
Cartelol	0.868049	0.088312	0.9360985	11
Cyclopentolate	0.828406	0.083254	0.8875452	10
Iodoxamide	0.669179	0.065523	0.7074112	5
Ganciclovir	0.666756	0.067637	0.7179592	6

Table 11. VIKOR ranking of ophthalmic drugs based on molar volume

Ophthalmic drugs	S_j	R_j	Q_j	**Molar volume rank**
Acetazolamide	0.297575	0.035330	0.3297500	2
Acetylcysteine	0.000000	0.000000	0.0000000	1
Aciclovir	0.535419	0.062463	0.5877380	4
Tropicamide	0.766094	0.083981	0.8133848	9
Xylometazoline	0.710151	0.079877	0.7643475	8
Apraclonidine	0.463231	0.048558	0.4804811	3
Brinzolamide	0.996071	0.095238	0.9863080	12
Bromfenac	0.719843	0.076367	0.7512919	7
Cartelol	0.866037	0.086021	0.8739701	10
Cyclopentolate	0.831103	0.097919	0.9171902	11
Iodoxamide	0.671122	0.066966	0.6788280	6
Ganciclovir	0.668227	0.067169	0.6784134	5

Table 12. VIKOR ranking of ophthalmic drugs based on molar refractivity

Ophthalmic drugs	S_j	R_j	Q_j	**Molar refractivity rank**
Acetazolamide	0.305659	0.039021	0.3835859	2
Acetylcysteine	0.000000	0.000000	0.0000000	1
Aciclovir	0.533018	0.055406	0.5945314	4
Tropicamide	0.760831	0.082356	0.8678717	9
Xylometazoline	0.705582	0.073039	0.7852226	7
Apraclonidine	0.460946	0.048843	0.5196086	3
Brinzolamide	0.992516	0.084975	1.0000000	12
Bromfenac	0.715700	0.076816	0.8125378	8
Cartelol	0.860836	0.084970	0.9336320	11
Cyclopentolate	0.825830	0.083163	0.9053644	10
Iodoxamide	0.667183	0.065496	0.7215320	5
Ganciclovir	0.664989	0.067563	0.7324594	6

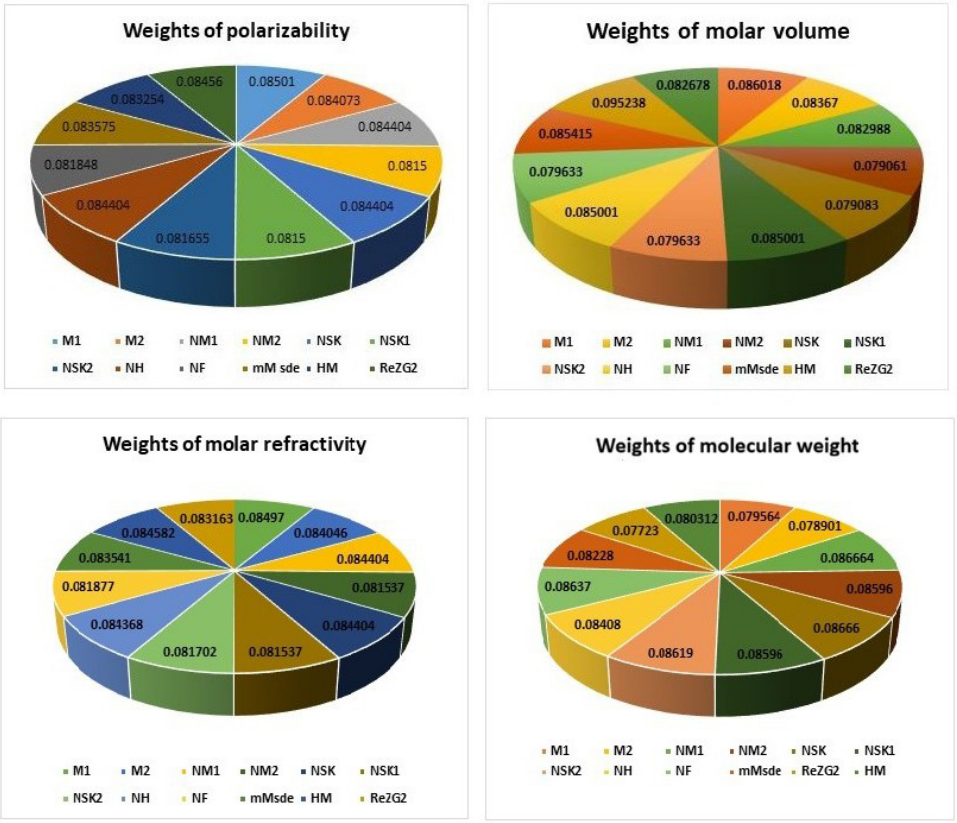

Figure 3. Weights of physicochemical properties of ophthalmic drugs

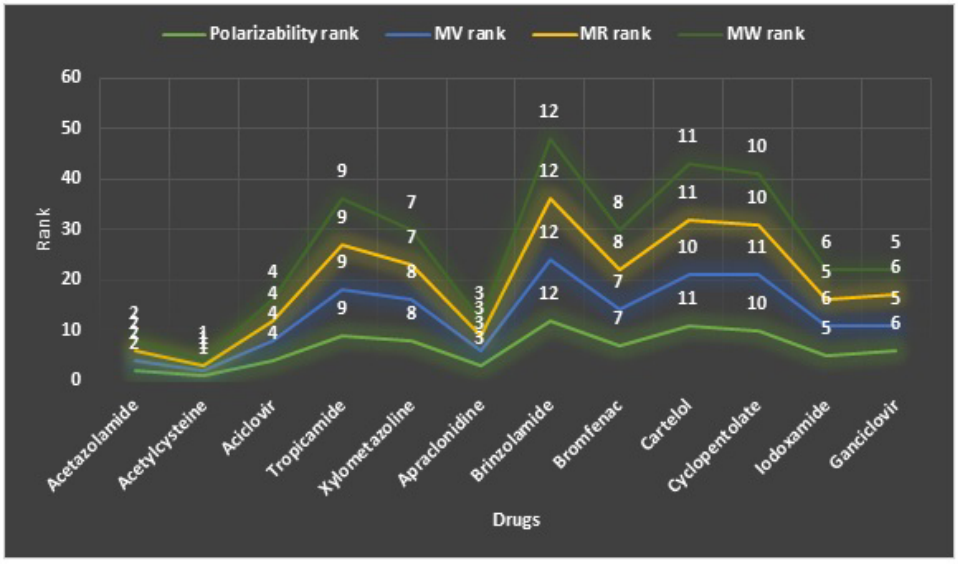

Figure 4. VIKOR ranking of Ophthalmic drugs based on molecular weight
Abbreviations: MR: Molar refractivity; MV: Molar volume; MW: Molecular weight

an antioxidant. Additionally, its well-established mucolytic agent aligns with high desirability in MCDM analysis, reinforcing its top ranking. Conversely, brinzolamide remains the least ranked candidate due to its higher molecular weight and complexity. Brinzolamide ranks last primarily because its heterocyclic and highly irregular graph topology creates uneven degree distributions and weaker performance in degree-based and Sombor-type topological indices, which favor structurally balanced molecules. Its specialized pharmacological use for glaucoma management limits its broader therapeutic desirability in multi-criteria ranking frameworks compared with drugs exhibiting wider clinical applicability. Additionally, the presence of multiple heteroatoms and rigid ring

Table 13. VIKOR ranking of eye drugs based on molar weight.

Ophthalmic drugs	S_j	R_j	Q_j	**Molecular weight**
Acetazolamide	0.294772	0.030830	0.3259944	2
Acetylcysteine	0.000000	0.000000	0.000000	1
Aciclovir	0.531909	0.051451	0.5641377	4
Tropicamide	0.757596	0.083069	0.8597464	9
Xylometazoline	0.702177	0.068569	0.7482064	7
Apraclonidine	0.459445	0.045396	0.4925774	3
Brinzolamide	0.995443	0.086666	1.0000000	12
Bromfenac	0.713226	0.071332	0.7697867	8
Cartelol	0.858819	0.082283	0.9060582	11
Cyclopentolate	0.818184	0.078024	0.8610233	10
Iodoxamide	0.665888	0.064510	0.7062766	6
Ganciclovir	0.663442	0.062739	0.6951228	5

Table 14. VIKOR ranking of ophthalmic drugs based on physicochemical properties

Ophthalmic drugs	P	MV	MR	MW
Acetazolamide	2	2	2	2
Acetylcysteine	1	1	1	1
Aciclovir	4	4	4	4
Tropicamide	9	9	9	9
Xylometazoline	8	8	7	7
Apraclonidine	3	3	3	3
Brinzolamide	12	12	12	12
Bromfenac	7	7	8	8
Cartelol	11	10	11	11
Cyclopentolate	10	11	10	10
Iodoxamide	5	6	5	6
Ganciclovir	6	5	6	5

Abbreviations: P: Polarizability; MR: Molar refractivity; MV: Molar volume; MW: Molecular weight.

systems reduces structural efficiency in graph descriptors, leading to lower scores beyond simple considerations of molecular weight. The stability of rankings in accordance with properties confirms the potency of VIKOR method in delivering a valid and compromise-based drug priority.

4. Conclusion

This study highlights that the combination of graph-theoretical topological indices with the QSPR modeling framework, and VIKOR-based MCDM analysis provides a reliable and systematic framework for the evaluation of ophthalmic drug candidates. The computed topological indices effectively capture slight divergences in molecular structure, supporting accurate prediction of key physicochemical properties such as polarizability, molar refractivity, molar volume, and molecular weight. The strong agreement between predicted and observed values confirms the robustness of the regression models and highlights the suitability of neighborhood-based indices in representing molecular behavior. The application of the VIKOR method further enhances the analysis by combining multiple physicochemical factors into a single compromise-based ranking scheme. The resulting hierarchy consistently identifies acetylcysteine as the most structurally efficient compound, reflecting its balanced molecular size, connectivity, and electronic characteristics.

Overall, the proposed computational framework reduces dependence on laboratory screening and offers a reproducible decision-support tool for early-stage drug evaluation. By connecting mathematical modeling with pharmaceutical analysis,

this approach contributes insights into drug priority and may be extended to other classes of remedial agents in future investigations.

Acknowledgments

None.

Funding

This work is funded by Faculty of Engineering and Quantity Surviving, INTI International University Colleges, Nilai, Malaysia.

Conflict of interest

The authors declare they have no competing interests.

Author contributions

Conceptualization: Muhammad Kamran, Shereen Iqbal, Hifza Iqbal, Muhammad Akhtar Tarar, Mohamad Hafez
Investigation: Shereen Iqbal, Hifza Iqbal, Muhammad Akhtar Tarar, Muhammad Kamran
Methodology: Shereen Iqbal, Hifza Iqbal, Muhammad Akhtar Tarar
Formal analysis: Muhammad Kamran, Muhammad Farman, Evren Hincal
Writing–original draft: Shereen Iqbal, Hifza Iqbal
Writing–review & editing: Muhammad Kamran, Muhammad Farman, Mohamad Hafez, Evren Hincal

Availability of data

Not applicable.

AI tools statement

All authors confirm that no AI tools were used in the preparation of this manuscript.

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Muhammad Kamran *holds multiple academic affiliations, serving as an adjunct faculty member at International Center for Interdisciplinary Research in Sciences, The University of Lahore, Lahore, Pakistan. His research is dedicated to fuzzy logics, graph-based networks, and intelligent systems.*
https://orcid.org/0009-0000-5467-0497

Shereen Iqbal *is a Ph.D. scholar in the Department of Mathematics and Statistics at The University of Lahore, Pakistan. Her current research interests lie at the intersection of chemical graph theory, QSPR analysis, and the application of machine learning techniques. She holds an M.Phil. degree, during which her work focused on mathematical inequalities.*
https://orcid.org/0009-0006-0734-1184

Hifza Iqbal *completed her Ph.D. at The University of Lahore, Pakistan, in 2021. She is currently serving as an Assistant Professor in the Department of Mathematics and Statistics at the same institution. Her research interests are primarily in graph theory and computational wave propagation.*
https://orcid.org/0009-0009-1614-9110

Muhammad Akhtar Tarar *is Associate Professor (Civil Engineering) at The University of Lahore, Lahore, Pakistan.*
https://orcid.org/0009-0008-6788-0870

Muhammad Farman *did Ph.D. Mathematics from the University of Lahore in 2019, Pakistan, and a Postdoc fellowship from Universitas Airlangga Indonesia, Lebanese American University, and Near East University, North Cyprus, Turkey. Adjunct Professor (Research), at Universitas Airlangga Indonesia and University of Lahore, Pakistan. Currently, he is working as an Associate Professor Dr. at Near East University. He has more than eight years of teaching and research experience. The research field is Mathematical biology, Control theory, Numerical Analysis, and Application of fractional calculus on Epidemic models. He published more than three hundred research papers in well-reputed SCI and Scopus journals and presented his work at several national and international conferences. He is the winner of several awards, such as the Research Excellent Awards (Best Researcher of the University), in 2019 and 2020 at the University of Lahore. Stanford University's Top 2% Scientists of 203, 2024 in Applied Mathematics. Best Academic Performance Award 2024, Publication Honorary Award 2024, Most Impactful Researcher Award 2024, Near East University, 2024.*
https://orcid.org/0000-0001-7616-0500

Evren Hincal *is a Professor at the Mathematics Research Center, Department of Mathematics, Near East University, Mersin, Turkey. His research focuses on computational mathematics.*
https://orcid.org/0000-0001-6175-1455

Mohamad Hafez *is a Professor at the Faculty of Engineering and Quantity Surveying, INTI International University Colleges, Nilai, Negeri Sembilan, Malaysia. His research focuses on sustainability and various other applications of mathematics.*